

Supporting Information

Unlocking Efficiency of Nonaqueous Li-Air Batteries through Synergistic Effect of Dual Metal Site Catalysts: An Interpretable Machine Learning Approach

Nishchal Bharadwaj,^a Surya Sekhar Manna,^a Milan Kumar Jena,^a Diptendu Roy,^a and Biswarup Pathak^{a*}

^aDepartment of Chemistry, Indian Institute of Technology (IIT) Indore, Indore, Madhya Pradesh, 453552, India

*E-mail: biswarup@iiti.ac.in

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Text S1. Details of density functional theory (DFT) calculations

All spin-polarized DFT computations are carried out using the Vienna Ab initio Simulation Package (VASP)¹ with the implementation of the projector-augmented wave (PAW) method.² The generalized gradient approximation of Perdew–Burke–Ernzerhof (GGA-PBE)³ is used to describe the exchange–correlation potential. Electronic wave functions are expanded by plane-wave basis sets with a kinetic energy cut off of 450 eV. All the DMSCs have been optimized in cubic box of 30 x 30 x 30 Å³ by maintaining a minimum distance of 10 Å between the periodic images to rule out their interactions. Gamma centered (1 x 1 x 1) k-point grid is considered for Brillouin zone sampling. The convergence criterion of 10⁻⁴ eV and < 0.02 eVÅ⁻¹ are employed for energy and atomic forces, respectively during the optimization of DMSCs. All the calculation parameters such as k-point grid, energy cutoff are verified for their convergence. The DFT-D3 method is used to take into account the van der Waals interactions.⁴ Further, to investigate the charge transfer processes, a Bader charge analysis has been performed.⁵

The adsorption energy of the intermediate is calculated by using the following equation,

$$E_{ads} = E_{DMSC + LiO_2} - (E_{DMSC} + E_{LiO_2})$$

where, $E_{DMSC + LiO_2}$ is the total optimized energy of DMSC with adsorbed LiO₂. E_{DMSC} and E_{LiO_2} are the single-point energies of DMSC and LiO₂, respectively.

Text S2. Details of considered machine learning algorithms.

XGBR Algorithm

XGBoost regression (XGBR) is a supervised learning method tailored for forecasting continuous numeric outcomes. Given a training set of N instances, each with M input features (x_1, x_2, \dots, x_M) , and a corresponding numeric output y , XGBR seeks to learn a predictive function $F(x)$ capable of accurately foretelling y for new inputs. In XGBR, $F(x)$ is shaped by combining T distinct decision trees. These trees, contributing individual predictions $f_t(x)$ for an input, coalesce into the final prediction through a weighted summation process,

$$F(x) = \sum_{t=1}^T f_t(x)$$

XGBR aims to identify the ideal set of decision trees $\{f_t\}$ that minimizes the loss function $L(y, F(x))$ without succumbing to overfitting. This is accomplished through a gradient-based optimization approach, progressively introducing new trees that diminish the difference between the true output and the current prediction. The optimization objective is framed as follows,

$$Obj(\Theta) = L(y, F(x)) + \Omega(\Theta)$$

In each iteration of XGBR, the aim is to discover the optimal model parameters Θ by minimizing the loss function $L(y, F(x))$ while considering model complexity through $\Omega(\Theta)$. Through successive steps, XGBR calculates the negative gradient of the loss concerning the current prediction, leveraging it as the next tree's target. The new tree is incorporated into the ensemble by determining the best split point, maximizing the reduction in the objective function.

In essence, XGBR stands as a potent and adaptable algorithm, effectively applicable across diverse regression scenarios, showcasing exceptional performance on benchmark datasets and attaining leading-edge outcomes.

ADR Algorithm

AdaBoost regression (ADR) amalgamates multiple weak learners to construct a robust predictor.

This mathematical concept can be elucidated through the subsequent key points:

1. At the outset, initialize the weight of each training sample as $w_i = 1/N$, where N is the total number of training samples.
2. For each iteration $t= 1,2, 3,\dots,T$
 - a. Train a weak learner on the training data with the current weights.
 - b. Calculate the error of the weak learner (ϵ_t),

$$\epsilon_t = \frac{\sum (w_i * |(y_i - f_t(x_i))|)}{\sum w_i}$$

Where, y_i is the target value for the i^{th} training sample, $f_t(x_i)$ is the prediction of the weak learner for the i^{th} sample, and $\sum w_i$ is the sum of weights over all training samples.

- a. Further, calculate the weight of the weak learner (α_t),

$$\alpha_t = \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$

- b. Instantly, update the previous training sample (w_i),

$$w_i = w_i * e^{\alpha_t |(y_i - f_t(x_i))|}$$

1. The ultimate predictor materializes as the weighted fusion of the weak learners, with the weight of each learner being directly linked to its alpha value.

KRR Algorithm

Kernel ridge regression (KRR) stands as a valuable supervised learning technique designed primarily for regression tasks. While bearing resemblance to the conventional ridge regression approach, KRR distinguishes itself through the incorporation of a non-linear transformation applied to the input data. This transformation occurs within an augmented dimensional realm referred to as the feature space, all facilitated by the utilization of a kernel function. The essence of this transformation lies in its capability to facilitate the capture of intricate and nuanced connections that may exist between the input variables and the target variable. In essence, KRR harnesses the power of kernel functions to elevate its regression capabilities beyond linear constraints, enabling it to navigate and model intricate relationships within the data.

KRR consists of the goal to find a function $f(x)$ that maps the input variables x to the target variable y , given a set of training data (x_i, y_i) , where $i = 1, 2, \dots, n$. The function $f(x)$ is a linear combination of the kernel functions $K(x, x')$ evaluated at the training data points x_i ,

$$f(x) = \sum_{i=1}^n \alpha_i * K(x, x_i)$$

Here, α_i are the coefficients of the linear combination.

In kernel ridge regression (KRR), the kernel function's selection holds significance, as it dictates the non-linear conversion of input data to a higher-dimensional feature space. Typical kernels encompass the linear, polynomial, radial basis function (RBF), and sigmoid types. In essence, KRR is a potent method, leveraging kernel functions to map data to an elevated dimensional realm, enabling the capture of intricate associations between input and target variables.

GBR Algorithm

Gradient boosted regression (GBR) emerges as a comprehensive ML model, resulting from the fusion of weak regression trees. In the presence of training samples $D = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$, each regression tree $t_m(x)$ is characterized by J leaf nodes, defining J distinct regions within the input data. The training objective of GBR revolves around minimizing the loss function L , shaping decision tree parameters θ_m via empirical risk minimization.

$$\theta_m = \sum_{i=1}^n L(y_i f_{(m-1)}(x_i) + t_m(x_i))$$

The process of GBR training is as follows:

- (a) At the outset, the Initialization of a regression tree function $f_0(x)$.
- (b) Train GBR in the gradient decline direction and compute the negative gradient value of the loss function as the estimated value of the residual. For the m^{th} iteration, GBR generates a regression tree according to the residual and updates the current function $f_m(x)$.
- (c) The final regression model is the weighted sum of several weak regression trees, which is defined as:

$$f_M(x) = \sum_{m=1}^M t(x, \theta_m)$$

ETR and RFR Algorithms

The extra tree regression (ETR) technique evolved from the original random forest (RF) model. In ETR's conventional top-down strategy, a set of unpruned decision or regression trees is built. In random forest regression (RFR), the process entails two phases: bootstrapping and bagging. Bootstrapping yields a collection of trees, each grown with a random training dataset sample. The

subsequent bagging step further refines tree nodes through multiple random subsets of the training data.

For RFR's decision-making, optimal subsets and their values are selected iteratively. The approach incorporates a sequence of decision trees, denoted as predicting trees. An independent distribution vector is denoted as is assigned before each tree's growth. All trees amalgamate into an ensemble (forest), with their outputs averaged according to a specific equation.

$$G(x, \theta_1, \dots, \theta_r) = \frac{1}{R} \sum_{r=1}^R G(x, \theta_r)$$

There are differences between ETR and RFR such as,

1. In ETR, all the cutting points are employed for node division, with nodes being split through random selection from these points.
2. It uses the entire learning samples to cultivate the trees to minimize bias.

DTR Algorithm

Decision tree regression (DTR) operates by iteratively segmenting the feature space into distinct regions and fitting uncomplicated models (often constants) within each region. The outcome of a decision tree regression is expressed by the subsequent equation:

$$y = \sum C_i * I(x \in R_i)$$

where y is the predicted output value, C_i is the constant value for region i , and $I(x \in R_i)$ is an indicator function that returns 1 if the input x belongs to region i , and 0 otherwise. The regions R_i Here y is the predicted output value, C_i is the constant value for region i , and $I(x \in R_i)$ is an indicator function that returns 1 if the input x belongs to region i , and 0 otherwise. The region R_i is defined by the splits in the decision tree, which are based on the values of the input features.

The objective of the decision tree regression algorithm is to identify optimal splits that minimize the mean squared error between predicted values and actual values within the training dataset.

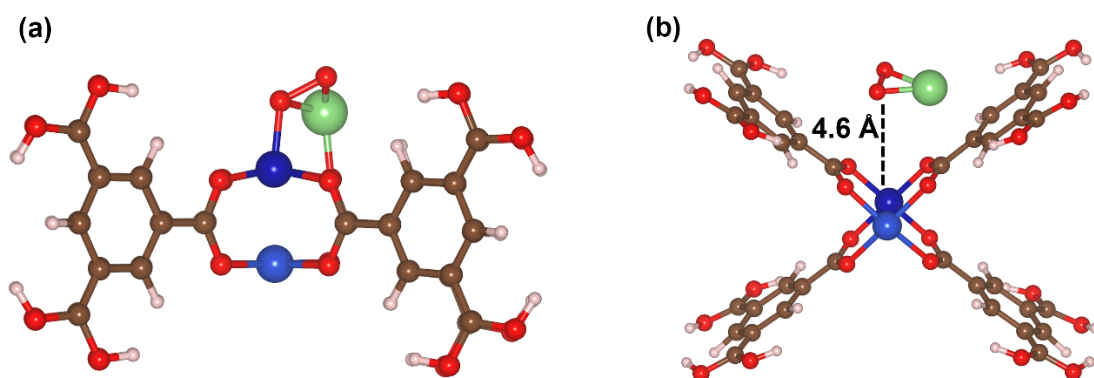


Figure S1. The optimized structures of possible sites of DMSCs for LiO_2 adsorption. (a) Top site and (b) bridge site.

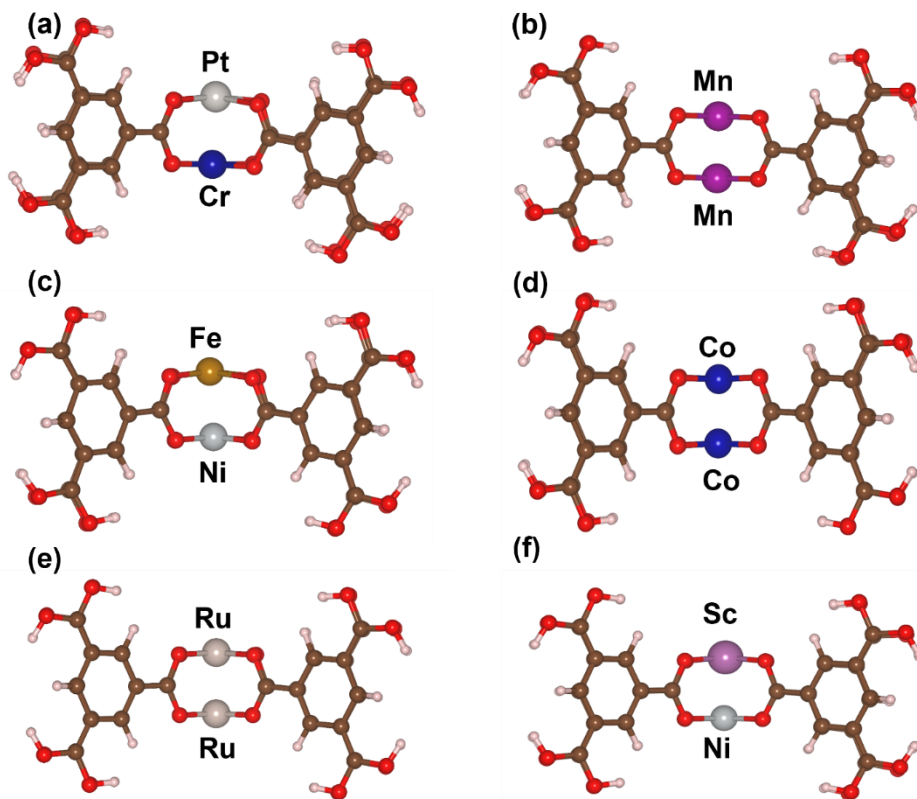


Figure S2. The optimized structures of some representative DMSCs. Here, brown, red, and pink colors represent C, O, and H atoms, respectively.

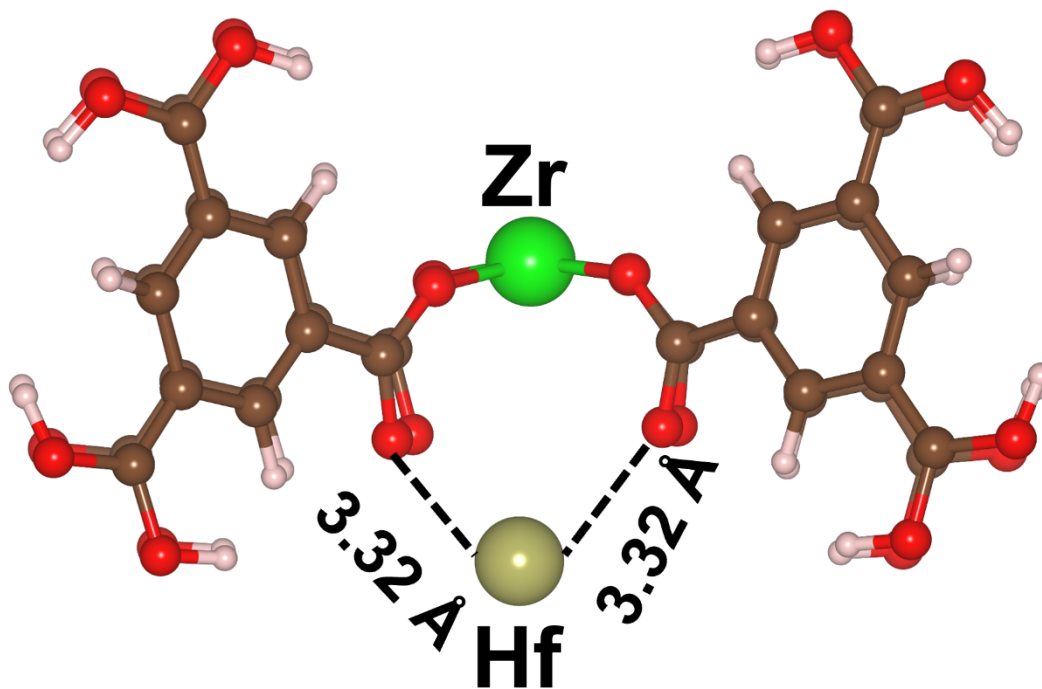


Figure S3. The optimized structures of DMSCs consist of Zr and Hf elements. The Dotted line shows a weak interaction of the BTC ligand with Hf.

Text S3. Calculation of the number of possible combinations within DMSCs

The calculation of the number of possible metal combinations within DMSCs for all the considered transition metal:

$$n_{Cr} = \frac{n!}{r! * (n - r)!}$$

Total number of considered transition metal = 26,

$$\text{Hence, total heteronuclear combinations for two metal sets} = {}^{26}C_2 = \frac{26 * 25 * 24!}{2! * 24!} = 325$$

Since both metals can act as active sites, the total adsorption sites = 2 x 325 = 650

Total homonuclear metal combinations for DMSCs = 26

Therefore, the total number of possible combinations: 650+26=676

Table S1. Optimized Set of Features Corresponding to Lowest MAE

Features	$N_{d1}, \aleph_{P1}, \aleph_{P2}, \aleph_{M1}, N_{d1} + N_{d2}, N_{d1} - N_{d2}, N_{d1} \times \aleph_{P1},$ $\aleph_{P1} \times \aleph_{P2}, \aleph_{M1} \times \aleph_{M2}, N_{d1} \times \aleph_{M2}, N_{d1} \times \aleph_{M1}, \aleph_{P1} - \aleph_{P2},$ $\aleph_{M1} - \aleph_{M2}, \text{avg. atomic radius in } \text{\AA} (\bar{r}_a), \text{ avg. ionic radius in } \text{\AA}$ $(\bar{r}_i), \text{ avg. crystal radius in } \text{\AA} (\bar{r}_c), \text{ avg. Mulliken electronegativity}$
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	(\bar{N}_M)
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Table S2. The Details of Optimized Hyperparameter Values and Their Corresponding Train-Test Mean Absolute Error (MAE) Scores for Considered Seven Machine Learning Regression Models

Sl. No.	Models	Hyperparameters	Train MAE (eV)	Test MAE (eV)
1	XGBR	cv=3, learning_rate=0.05, max_depth=25, min_child_weight=2, n_estimators=100, objective='reg:squared error'	0.04	0.13
2	ADR	learning_rate=0.1, loss='exponential', n_estimators=1400	0.10	0.14
3	KRR	alpha=0.01, coef0=4, gamma=0.001, kernel='laplacian'	0.11	0.13
4	GBR	alpha=0.08, max_depth=10, learning_rate=0.06, n_estimators=200, verbose=40, min_samples_leaf=10	0.09	0.13
5	ETR	max_depth=4, max_features=13, max_leaf_nodes=15, min_samples_leaf=4, min_samples_split=4	0.16	0.14
6	DTR	max_depth=7, max_features='auto', min_samples_leaf=8, min_weight_fraction_leaf=0.1, splitter='random'	0.18	0.14
7	RFR	max_depth=20, min_samples_leaf=5, min_samples_split=3, n_estimators=200	0.11	0.17

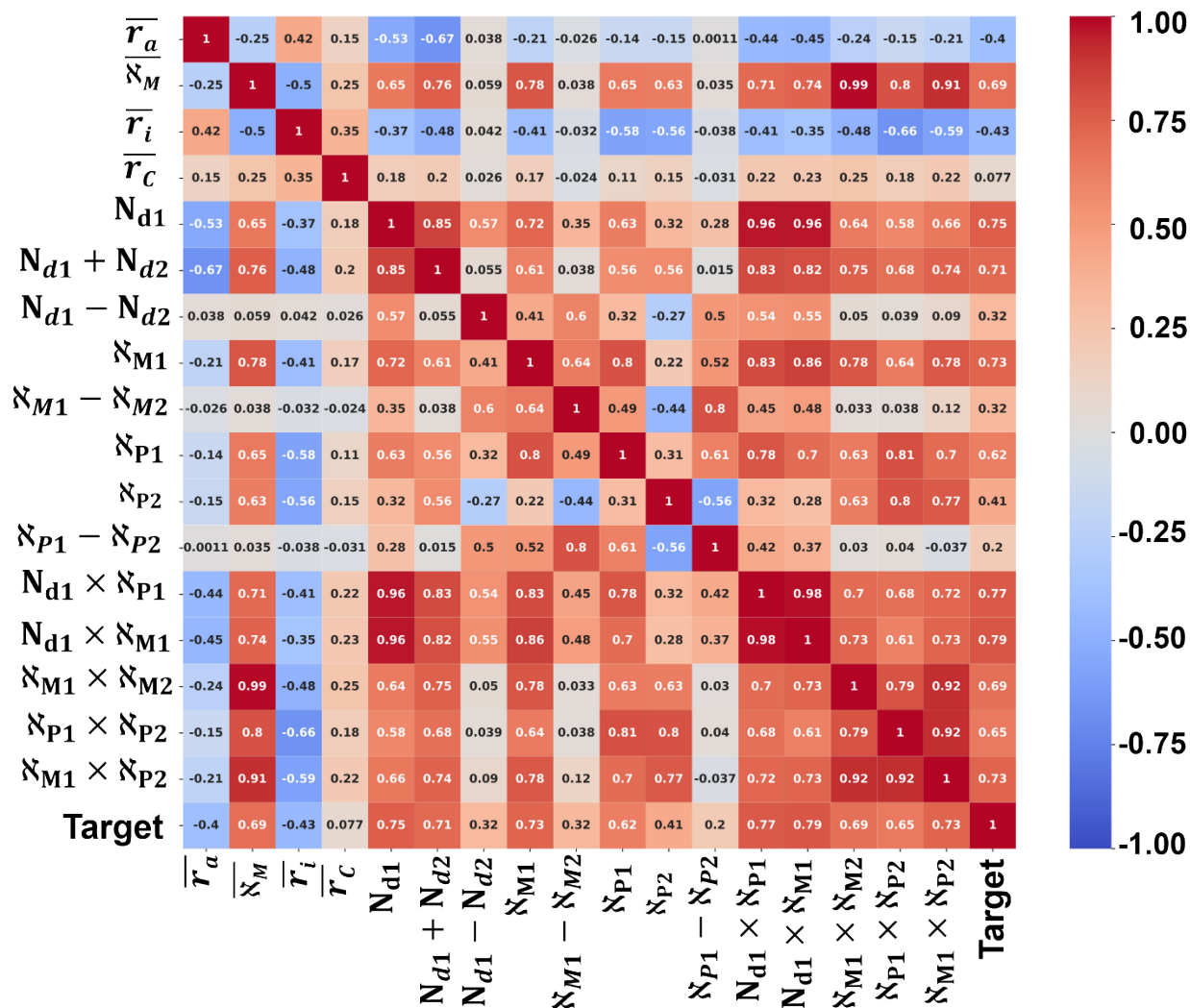


Figure S4. Pearson's correlation coefficient (PCC) analysis between final set of features and the target variable (adsorption energy). The color scale on the right side indicates the correlation strength, with dark red indicating a strong positive correlation and dark blue representing a strong negative correlation.

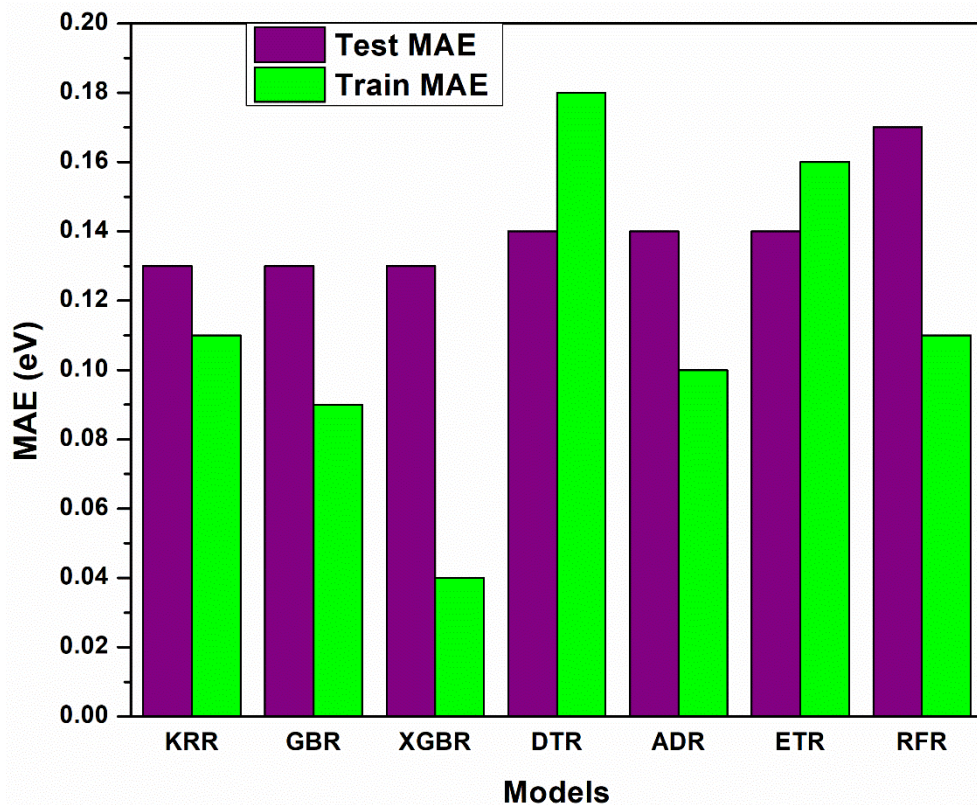


Figure S5. Bar plots representing train and test errors for all the considered models.

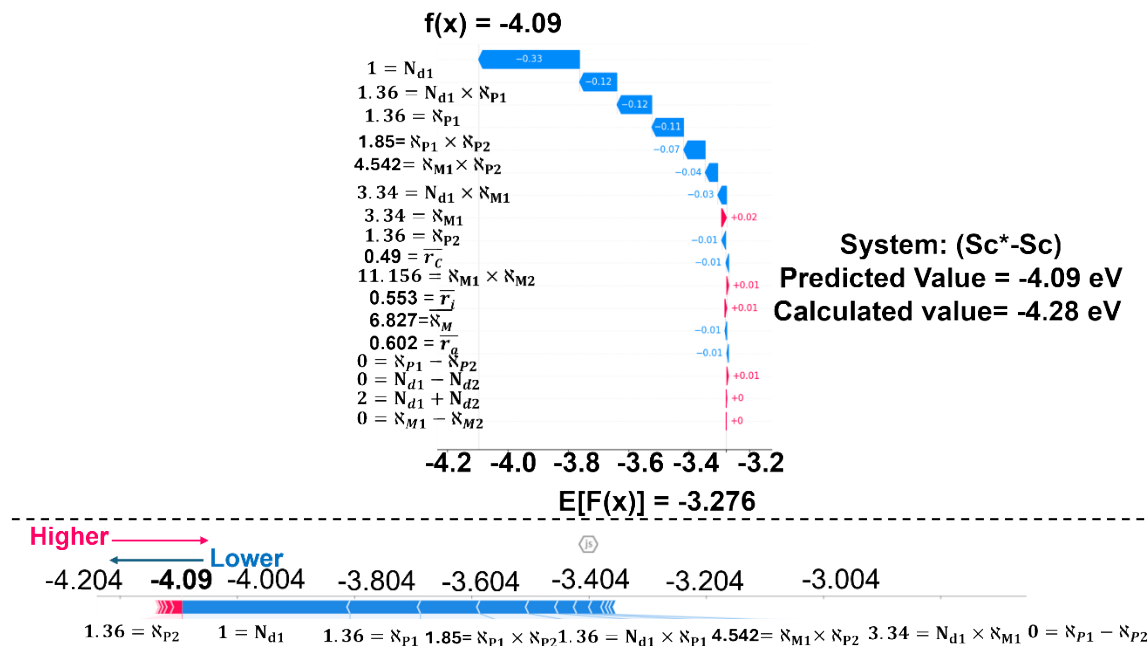


Figure S6. SHAP waterfall plot visualizing the contribution direction of the individual feature for the most deviated system of Sc^{*}-Sc based DMSC.

Text S4. Calculation of the LiO₂ solvation energy within an explicit DMSO environment

The solvation energy of LiO₂ is calculated as follows,

$$\text{Solvation energy} = E_{DMSO_LiO_2} - E_{DMSO} - E_{LiO_2}$$

where, $E_{DMSO_LiO_2}$, and E_{DMSO} are the total energy of LiO₂ with explicit DMSO solvent and bulk DMSO solvent system without LiO₂ molecule, respectively. E_{LiO_2} is the total energy of an isolated LiO₂ molecule.

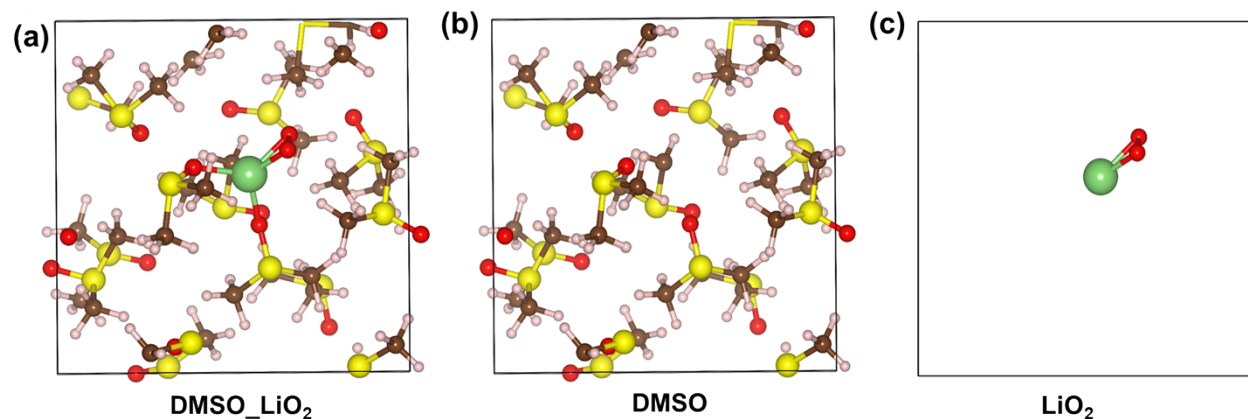


Figure S7. Optimized structures of (a) LiO₂ with explicit DMSO solvent, (b) DMSO solvent without LiO₂, and (c) isolated LiO₂ molecule. Green, red, yellow brown, and pink color represent the lithium, oxygen, sulfur, carbon, and hydrogen atoms, respectively.

Text S5. Calculation of the charge density difference plots for LiO₂ adsorbed DMSCs

The charge density difference is calculated as follows,

$$\Delta\rho = \rho_{LiO_2_DMSC} - \rho_{DMSC} - \rho_{LiO_2}$$

Here, ρ_{LiO_2-DMSC} , ρ_{DMSC} , and ρ_{LiO_2} are the total charge densities of the LiO_2-DMSC , DMSC without LiO_2 , and isolated LiO_2 molecule, respectively.

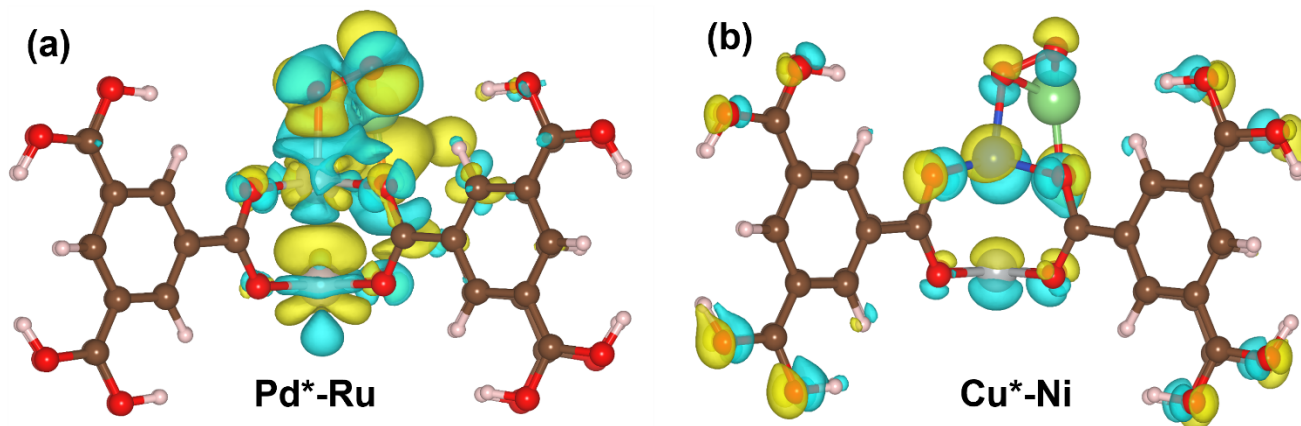


Figure S8. The charge density difference plots of LiO_2 adsorbed on (a) Pd^*-Ru DMSC (isosurface = 0.007 eV/\AA^3) and (b) Cu^*-Ni DMSC (isosurface = 0.08 eV/\AA^3). The yellow and cyan colors indicate electron density accumulation and depletion, respectively.

Text S6. Coordinates of the structures considered in this study.

Ru*-Ru DMSC

```
1.0000000000000000
30.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000
```

```
Ru O C Li H
2 26 36 1 28
```

Direct

```
0.5060486593742873 0.5113605602704696 0.5395180491948578
0.4916202571133489 0.4906863027377561 0.4673944663211720
0.3271455209720276 0.4729422654465951 0.6765834845086017
0.2806944855047552 0.4025022917432954 0.4457699409363107
0.3776575525633112 0.6516536424568466 0.3510802356377675
0.4243826414542920 0.7225092718960235 0.5817463047184429
0.2249921679831304 0.4095935796975348 0.4934920186726200
0.4772532359597307 0.5728475751381161 0.5262315341640774
```

0.4444420056714231 0.4884490205232035 0.5578142917316972
0.3413755431769286 0.7090929174497658 0.3796100769904478
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0.4629958615881697 0.5513595707653899 0.4552143277648775
0.2581260813597877 0.4576474435303503 0.6564211633154857
0.5694899573154831 0.5355896356313660 0.5178005355471076
0.5355121951571467 0.4497764962540617 0.5491266209623150
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0.5532956767881140 0.5129909643779813 0.4479673950974450
0.7333963705034068 0.5368767043925424 0.3390476223630529
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0.6582380582120748 0.2877444148334589 0.6163873738229714
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0.3589968923905444 0.4660866410535801 0.5846784125512098
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0.3876554229009223 0.7012171169334606 0.4647716646025061
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0.5658179513481676 0.3505671505459751 0.4867084660164024
0.5824127941960709 0.3706927078150870 0.5637516266249358

0.6806612400074892 0.5438284941742045 0.4005459733569650
 0.7017862590021393 0.5681671260277738 0.4768354702822414
 0.5909260186425055 0.3103399609975144 0.4908466285495676
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 0.6916128216749892 0.5356204892836630 0.3557308088169588
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 0.7336943240843479 0.5846400384280803 0.5069386618852147
 0.5952664475722111 0.2814859536884329 0.4541104186902433
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 0.3556095044554324 0.4411234441574326 0.4740420577406567
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 0.6322809865753697 0.5302372120382495 0.3341282439129217

Pd*-Pd DMSC

1.0000000000000000
 30.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 30.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 30.0000000000000000

Pd O C Li H

2 26 36 1 28

Direct

0.4856816206957644	0.5385875199678622	0.5933533907639755
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Ir Cr O C Li H
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Pt Fe O C Li H

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Co*-Fe DMSC

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Co Fe O C Li H

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Ni Fe O C Li H

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Ni*-Pd DMSC

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Pd Ni O C Li H

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Pd*-Ni DMSC

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Pd Ni O C Li H

1 1 26 36 1 28

Direct

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0.3770832289934112	0.6521224865079472	0.3505030860480693
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0.2249203666921673	0.4098630024815236	0.4934276038548732
0.4788158510695781	0.5732917729282251	0.5259458466023913
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Pd	Cu	O	C	Li	H
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Direct

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0.2780486877994235	0.4012985158996586	0.4447155918663138
0.3785167175454525	0.6505812890739584	0.3513129780661802
0.4246260363110174	0.7225746428595742	0.5813430180897448

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Pd*-Cu DMSC

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Pd Cu O C Li H
1 1 26 36 1 28

Direct

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Ru*-Rh DMSC

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Rh Ru O C Li H

1 1 26 36 1 28

Direct

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Rh Ru O C Li H

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Pt*-Ru DMSC

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Direct

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0.4248651073976442	0.7219112434606098	0.5819400225529759
0.2256738519680711	0.4098120496409542	0.4937843258882857
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Ir*-Pt DMSC

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Pt Ir O C Li H

1 1 26 36 1 28

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Y Zn O C Li H
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Mo*-Re

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Re Mo O C Li H

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0.5806712802848695 0.3948235307443320 0.5905107007517268

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Rh* -V DMSC

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Rh V O C Li H

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Pd*-Cr DMSC

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Pd Cr O C Li H

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Cd*-Mn

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 Cd Mn O C Li H
 1 1 26 36 1 28

Direct

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Nb*-V

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Nb V O C H
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Direct

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Co*-Au

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 Au Co O C Li H
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Direct

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Ni*-Cu

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Cu Ni O C Li H
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Direct

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0.6126998152050179 0.5209374946896178 0.3981477629844393
0.6498749269168156 0.5603318768611757 0.5252953268302730
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0.7429707128012231 0.5747331508666327 0.4189869976290621
0.6240232212066376 0.2672571034799172 0.5384461894545064
0.3292241450224782 0.7194975910478019 0.4071785363314582
0.2162623159519163 0.4278516431978517 0.5191433012818808
0.4023543933825062 0.6339193528797197 0.3556779698326196
0.3124079632626171 0.4010953161637603 0.4443395985227592
0.5485728257667640 0.3071950881182450 0.4200036696700842
0.7552662151535623 0.5344261283293599 0.3650718372358794
0.6470581578034901 0.2508060354406109 0.4758573703613836
0.5976616249064697 0.3599186342937134 0.6473395915308615

0.6714406578453070 0.2775929307511258 0.5870230569545617
0.7852738062191431 0.5678017831054525 0.4734037837669893
0.6919397837292325 0.6070503820316876 0.5521995552463016
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0.2389670158467453 0.4586872770114070 0.6316630947891309
0.3539656868340968 0.7554013960329033 0.5191279463346479
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0.6325274556119057 0.5297738929430762 0.3347097583441330

Mn*-Re

1.0000000000000000

30.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000

Re Mn O C Li H
1 1 26 36 1 28

Direct

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0.2845618446532364 0.4051263530270525 0.4499403477473099
0.3792639924909097 0.6510799845863090 0.3553993508356939
0.4260791901329081 0.7240770550313907 0.5853487321311565
0.2285340716631094 0.4119426544397601 0.4972762645890098
0.4793538089437867 0.5724250485634338 0.5302297264891881
0.4486891582239264 0.4907451271993083 0.5614263973915892
0.3427368960858812 0.7085953739216598 0.3831963627980659
0.3757016443803604 0.7600261409539301 0.5452623478090581
0.4325282966525820 0.4688760495064719 0.4908110852752275
0.4647129643379174 0.5521847602939851 0.4592242759138616
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0.5373190121857095 0.4523529852196999 0.5527094052726589
0.5205196562162434 0.4311767463684812 0.4819822951884615
0.5526959708412427 0.5135358435099044 0.4496047892172284
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0.7227004402996959 0.6002839944051206 0.5531293262736554
0.7756442977256449 0.5892292538326604 0.5032430650201061
0.5728862336512708 0.2874324670258183 0.4190270647335080
0.6236391589084042 0.2483841372045133 0.4554583771145223
0.6590749061745623 0.2891135343492234 0.6200719206047629
0.6231831435756402 0.3445966238292872 0.6525442365564138
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0.5195286370138199 0.5315065721592788 0.6033643929663510
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0.3860374319154309 0.4823525335492566 0.6129481088229566
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0.4483464138104795 0.6466168839200449 0.5503730981963297
0.2564200289911983 0.4243262780783039 0.5801159875548234
0.3757953087766162 0.7345883434410756 0.4609008725289055
0.6116807688220881 0.5184597725760980 0.3987776843385055
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0.5809141171580154 0.3972608257389831 0.5940654863901911
0.7433600810927807 0.5755660499423801 0.4230204746159758

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0.3310491683644456	0.7198526614709365	0.4114291340284250
0.2194361867804654	0.4294576880700368	0.5231517161569997
0.4051919040781284	0.6320238779347445	0.3604534678239747
0.3170151777158854	0.4034019623717154	0.4483521238917598
0.5491061674586183	0.3092437199681978	0.4232660137984022
0.7548437157434216	0.5361928131870457	0.3680386771722750
0.6462089008748405	0.2516638914626786	0.4786613590063167
0.5976268821557424	0.3644724504422880	0.6493415107616781
0.6700600917024446	0.2799075423305297	0.5908345410492861
0.7825867685867044	0.5702796084854463	0.4776973597274936
0.6904880018208679	0.6028803344280024	0.5568758622252177
0.3608706593501801	0.4695171127938447	0.6727441972917225
0.2415053959484670	0.4605274771355992	0.6343516298863556
0.3535807321217715	0.7546935517024813	0.5219743580186124
0.4531056694086040	0.7063789628954031	0.5818609281877879
0.6328993379534716	0.5299757440615898	0.3381551008804416

Ni*-Pt

1.0000000000000000

30.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 30.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

Pt Ni O C H

1 1 24 36 28

Direct

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0.2885861513284921	0.3991122890189190	0.4426066311959823
0.3850828582431219	0.6499427992819262	0.3514648577542798
0.4252728802536893	0.7278113080243653	0.5808511575907357
0.2304254883153994	0.4041584443823371	0.4875900855240767
0.4785642659811539	0.5739971351651048	0.5300817443564348
0.4451961204107560	0.4900815373941035	0.5607645606736493
0.3489909425590964	0.7092322085880070	0.3762428832410682
0.3775454923835190	0.7637524538986264	0.5378197911779784
0.4311393048576346	0.4690627420329975	0.4887374332888166
0.4630056768564016	0.5524445600040142	0.4584542707718927
0.2533670130889790	0.4543601387701359	0.6509660805708682
0.5688278727266679	0.5364029311628318	0.5207207693661783
0.5359073489924995	0.4531156610037462	0.5527120865107619
0.5199240768135275	0.4324884810000434	0.4809352728356594
0.5510761297856289	0.5152934160462892	0.4495504289337235
0.7258234123866958	0.5357656741187313	0.3357389296327898
0.7256207115706077	0.6051259339717604	0.5437218570887793

0.7755374443611615 0.5930380409397634 0.4909048986271489
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0.4221228662995497 0.6024533789758746 0.4159436203268839
0.4465459747467647 0.6466851667206588 0.5487125895500310

0.2542395128332613	0.4182953208498040	0.5712001868244874
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0.6072445296565070	0.5169331721653740	0.3981010324267860
0.6466792010985329	0.5650414377543849	0.5259512998283827
0.5489796407448105	0.3644369989112397	0.4576761994292463
0.5824419060565658	0.3988670928268718	0.5914044299773447
0.7392403042665336	0.5757327781820762	0.4138490062295167
0.6217687231467013	0.2685150977050639	0.5393364218799330
0.3368105491121409	0.7216228352313377	0.4037719725242601
0.2197051400491967	0.4214683796804046	0.5129942032931868
0.4097764280853290	0.6298955778782092	0.3584388949899974
0.3211396576102975	0.3986468129966533	0.4423688686301046
0.5425315032698744	0.3096853056108710	0.4232317146047209
0.7481504600825089	0.5355454628681247	0.3594093855013253
0.6392845484953030	0.2495159431536768	0.4763489736484456
0.6013033212245841	0.3670219311213692	0.6461223295847361
0.6673343394034605	0.2775366024600289	0.5873349008949540
0.7813955462855917	0.5730055760637106	0.4659207030544560
0.6936624795823257	0.6086094737872011	0.5486916659428279
0.3525115203151382	0.4675883306854541	0.6681206992916829
0.2354483402466943	0.4554841142429071	0.6238054894075040
0.3561296390737326	0.7584015937344138	0.5139003173229980
0.4491731737593801	0.7057503025123437	0.5801839367894056
0.6248115538138156	0.5262560086742949	0.3368531554947069

Au*-Co

1.0000000000000000

30.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	30.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Au	Co	O	C	Li	H
1	1	26	36	1	28

Direct

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0.2997579669378932	0.4599142565955872	0.6652829240055458
0.3024734185150759	0.4010828904002381	0.4272122203910063
0.3933879276047595	0.6390364553924199	0.3660188550842968
0.4215376495121445	0.7350877123849351	0.5900645226624055
0.2388402975012720	0.3987514550687056	0.4641464943391004
0.4859380001507067	0.5819705287624991	0.5517670568268880
0.4283607739504778	0.5019477018655505	0.5721607315322628
0.3539658900620437	0.6982818634768937	0.3848060705170575
0.3738706908558731	0.7654949650733002	0.5430450939594904
0.4386133339802574	0.4719375107950222	0.5030694580781705

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0.2376273748560934 0.4367380527262298 0.6338738184133141
0.5756056485769431 0.5724275650602483 0.5114343704790063
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0.7127692823589582 0.5141359474054401 0.3222577656520523
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0.5802598776076395 0.5447741828185082 0.4800986546574152
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0.5489877856615173 0.5943356272927526 0.5611708825118916
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Cu*-Ni

1.0000000000000000
30.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000

Cu Ni O C Li H
1 1 26 36 1 28

Direct

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Cr*-Rh

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Rh Cr O C Li H
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Direct

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Au*-Ag

1.0000000000000000

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0.0000000000000000 30.0000000000000000 0.0000000000000000
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Au Ag O C Li H
1 1 26 36 1 28

Direct

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V*-Fe

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Fe V O C Li H

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Y*-Sc

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Y Sc O C Li H

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Ag*-Au

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Au Ag O C Li H
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Direct

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Mn*-Cd

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0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000

Cd Mn O C Li H
1 1 26 36 1 28

Direct

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Os*-Fe

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Os Fe O C Li H

1 1 26 36 1 28

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Y*-Ta

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Ta Y O C Li H

1 1 26 36 1 28

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W*-Ti

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W Ti O C Li H
 1 1 26 36 1 28

Direct

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Sc*-Cu

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Cu Sc O C Li H
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Pt*-Cu

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Pt Cu O C Li H
1 1 26 36 1 28

Direct

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0.7174213410356778 0.5603374228268915 0.4232664174039463
0.7409617250136917 0.5861332154143838 0.4979926357210245
0.5916881730104476 0.2843363350277058 0.4531919207278061
0.6100466690709380 0.2997433099574990 0.5316428924848082
0.6299235522359387 0.3172486028666556 0.6097962685704827
0.5673427433474364 0.5183802922185408 0.5665730047140859
0.3729240780553529 0.4744199412344388 0.6104332965554257
0.3536033495147459 0.4397749236466230 0.4742969580986933
0.4221094337818616 0.6018458186009890 0.4170013836549613
0.4442714579203006 0.6483865562490151 0.5483780085517881
0.2445526402301960 0.4202143381546498 0.5693258227045156
0.3729249418842556 0.7340285812317822 0.4540404991502587
0.6138355790398892 0.5189808304713416 0.3928436167622599
0.6540970885821865 0.5682895846454901 0.5191882412627409

0.5515464226458346	0.3665946289562552	0.4576922179933718
0.5903722146195294	0.3968372299097102	0.5904636456827270
0.7489834651476022	0.5717391210976317	0.4089565860439990
0.6212445250436280	0.2652936211222826	0.5358735327762194
0.3308772369623103	0.7175741175438313	0.4041494225214724
0.2109131204169075	0.4247183722026989	0.5115993381666585
0.4064469530289660	0.6279375443376006	0.3589399409109921
0.3123624437085269	0.3995605955202005	0.4417071351993455
0.5453502157463987	0.3121253028033122	0.4201511814710128
0.7563628679341836	0.5332506813720792	0.3552084449468110
0.6413526913653734	0.2504669069676947	0.4727899220491904
0.6020692848912842	0.3623950561761232	0.6443140857098627
0.6665810267140562	0.2710772653305362	0.5868066679138524
0.7909559339066472	0.5687815811011059	0.4631902463262851
0.7014822132132883	0.6040271925488064	0.5443052588505755
0.3454823894738500	0.4655263478272886	0.6667233831745758
0.2271672116868537	0.4542995763773644	0.6253649522852341
0.3528281110163620	0.7596190029820403	0.5129049596878147
0.4439024912223025	0.7043281361150178	0.5796077502842168
0.6330972321218257	0.5284312404520889	0.3308129864197155

Pd*-Ru

1.0000000000000000

30.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 30.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

Pd Ru O C H

1 1 24 36 28

Direct

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0.4911026646049731	0.4922500752710893	0.4690823245015704
0.3201299131306716	0.4700121876189390	0.6751389884549888
0.2875940811429335	0.3988724442527948	0.4425688420300244
0.3846956327116591	0.6501233831606392	0.3513947057677310
0.4250239332865140	0.7285486966498025	0.5803017215830604
0.2293632517755539	0.4037603924949787	0.4873099616225868
0.4782691305691318	0.5754023492732854	0.5310540993533952
0.4440282804642686	0.4891504973161758	0.5617246207494216
0.3488237110739776	0.7095605499296431	0.3758801585886044
0.3769831899782153	0.7646341221477440	0.5378446888364046
0.4308766328999281	0.4692164628557430	0.4893065865717081
0.4632198460999064	0.5530602241802020	0.4596498854550050
0.2523246871175739	0.4541407473606318	0.6514242590322732
0.5705280834531732	0.5379256569622746	0.5215238483224176
0.5364406429103576	0.4523317854412126	0.5539677918945852
0.5203276567123473	0.4327080979726032	0.4819933112752107

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0.3790831504822176 0.4804063426098983 0.6090787866337931

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0.4222389140489325	0.6027226589611047	0.4164076867251215
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0.2528082352879695	0.4182434865453023	0.5710381620296617
0.3785077460867004	0.7363014103391233	0.4546045441263790
0.6077950089022079	0.5169233796519563	0.3987314049078530
0.6482844656975592	0.5653565362687395	0.5257074147246715
0.5497571219184231	0.3644948866719209	0.4577880683307451
0.5830662433140893	0.3980204784979481	0.5913920879100706
0.7403218904074892	0.5754510426932213	0.4130690744913664
0.6224160268409582	0.2677395663824372	0.5388324853891305
0.3364080302734138	0.7220484353776901	0.4032516416006439
0.2183616485940718	0.4208115106210294	0.5127544620509531
0.4092590215653249	0.6299470246075943	0.3583873764056199
0.3201376676144824	0.3987279510973105	0.4423137478178612
0.5427921242003330	0.3094183688377137	0.4231664842531782
0.7484425654475820	0.5356353288549474	0.3585636812728790
0.6393329972694977	0.2486627187690743	0.4758720544649571
0.6017844735146579	0.3667777045012238	0.6451081730966935
0.6678522965365862	0.2765747684940211	0.5876789765863083
0.7830320541658662	0.5731253742566936	0.4655083825649040
0.6947214147479491	0.6083602612199086	0.5477586971306384
0.3515984734498820	0.4677705674186736	0.6671029916675342
0.2339647537985074	0.4550662883247512	0.6245737349248645
0.3555776112422736	0.7596029522325340	0.5138571932635726
0.4482833711515887	0.7057896744315564	0.5795401918309879
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Cu*-Au

1.0000000000000000

30.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	30.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Au Cu O C Li H

1 1 26 36 1 28

Direct

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0.2798449201113011	0.4007991526501111	0.4417049848697241
0.3814265594019332	0.6475400570158346	0.3518995805718017
0.4217185085434351	0.7282106229444389	0.5796735269090521
0.2216469067703714	0.4076607788658962	0.4860526530529490
0.4744128251044511	0.5780591340708496	0.5354571168189266
0.4374857308908577	0.4669512882522137	0.5732682398426573

0.3430717115736344 0.7051018257365080 0.3766720547235654
0.3733566039093802 0.7640166766625608 0.5377485288925780
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0.2457735674952845 0.4532334656445614 0.6519872643301087
0.5796049929326450 0.5512239371747870 0.5165057174856121
0.5639829680146632 0.4581291162402381 0.5493508479444388
0.5186781573955742 0.4371647618793139 0.4924144841147310
0.5566201813011454 0.5149534820831577 0.4543090373750273
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0.7335816719799420 0.6016715603077217 0.5393110164822024
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0.6181833601368958 0.2481073971833549 0.4500143575739644
0.6569199535791067 0.2818588862780727 0.6159349346574245
0.6252522695640748 0.3398060115541802 0.6481580394458919
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0.5716309463185013 0.5408542902681930 0.6257079269335150
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0.7079070863976279	0.5696323380761960	0.4687887378946327
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0.6932860192402173	0.5334926015099080	0.3495240945254341
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0.5916881730104476	0.2843363350277058	0.4531919207278061
0.6100466690709380	0.2997433099574990	0.5316428924848082
0.6299235522359387	0.3172486028666556	0.6097962685704827
0.5673427433474364	0.5183802922185408	0.5665730047140859
0.3729240780553529	0.4744199412344388	0.6104332965554257
0.3536033495147459	0.4397749236466230	0.4742969580986933
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0.2445526402301960	0.4202143381546498	0.5693258227045156
0.3729249418842556	0.7340285812317822	0.4540404991502587
0.6138355790398892	0.5189808304713416	0.3928436167622599
0.6540970885821865	0.5682895846454901	0.5191882412627409
0.5515464226458346	0.3665946289562552	0.4576922179933718
0.5903722146195294	0.3968372299097102	0.5904636456827270
0.7489834651476022	0.5717391210976317	0.4089565860439990
0.6212445250436280	0.2652936211222826	0.5358735327762194
0.3308772369623103	0.7175741175438313	0.4041494225214724
0.2109131204169075	0.4247183722026989	0.5115993381666585
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0.5453502157463987	0.3121253028033122	0.4201511814710128
0.7563628679341836	0.5332506813720792	0.3552084449468110
0.6413526913653734	0.2504669069676947	0.4727899220491904
0.6020692848912842	0.3623950561761232	0.6443140857098627
0.6665810267140562	0.2710772653305362	0.5868066679138524
0.7909559339066472	0.5687815811011059	0.4631902463262851
0.7014822132132883	0.6040271925488064	0.5443052588505755
0.3454823894738500	0.4655263478272886	0.6667233831745758
0.2271672116868537	0.4542995763773644	0.6253649522852341
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Pt*-Ni

1.0000000000000000

30.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	30.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Pt Ni O C H

1 1 24 36 28

Direct

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0.4252728802536893 0.7278113080243653 0.5808511575907357
0.2304254883153994 0.4041584443823371 0.4875900855240767
0.4785642659811539 0.5739971351651048 0.5300817443564348
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Mo*-Nb

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Mo Nb O C Li H
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Os V O C Li H

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0.5922236110694336 0.3112089128902855 0.4948801061455181
0.6090622182691826 0.3307705647902413 0.5735569981216666
0.6930548120932276 0.5362726202275432 0.3593946740653888
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0.7321638254627791 0.5857401445874225 0.5114384257388058
0.5964108131716070 0.2827934800491504 0.4578130579774932
0.6126448277561928 0.3008589303415054 0.5366203230335312

0.6301093505261910 0.3211358980294287 0.6143683341743474
 0.4828180642365774 0.5828085929349397 0.5908097696040072
 0.3848273792558801 0.4822059681814027 0.6130103957525083
 0.3581046126196183 0.4433250952100246 0.4788735474048287
 0.4190941248244361 0.6039629245808826 0.4176896779233246
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 0.2553651578830687 0.4240403947744684 0.5801944098180304
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 0.6125114093037706 0.5189662198272734 0.3981137390106896
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 0.5521853381778443 0.3623417939184810 0.4599761456046939
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 0.7444114209368810 0.5756365287862654 0.4227382928642471
 0.6260550582729724 0.2674016806602833 0.5420058169604917
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 0.4046795750114872 0.6329942782680097 0.3607846829772268
 0.3159253376301025 0.4029793759770915 0.4485984711405803
 0.5495777641680357 0.3084284178198412 0.4237638681637608
 0.7558679919615600 0.5362149470038218 0.3674639533369280
 0.6469158775325856 0.2507361952058832 0.4785601049603659
 0.5983967831753675 0.3632745677379960 0.6495283560346481
 0.6709804792808426 0.2788175147596209 0.5912205899611983
 0.7832710824012998 0.5703358362241984 0.4776316005699001
 0.6909812126619528 0.6029542116994920 0.5565596136418327
 0.3599962410235313 0.4688062751118434 0.6726815721204403
 0.2404193836221473 0.4604813878099007 0.6346354210839708
 0.3528152647660884 0.7559034496428384 0.5223458728640817
 0.4527656341670070 0.7076371732625774 0.5815758851859933
 0.6338415223154013 0.5302228533964406 0.3379693023111874

V*-Rh DMSC

1.0000000000000000

30.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 30.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 30.0000000000000000

Rh V O C Li H

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Direct

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 0.5089783561142950 0.5114135607851998 0.5412294001803877
 0.3293406398220317 0.4732888890021628 0.6811381874126503
 0.2832702702758352 0.4047761828486501 0.4496538976029160
 0.3790469702963504 0.6514782592892679 0.3551715924642167
 0.4262469019219150 0.7245279858315700 0.5849900698080891
 0.2273972408109069 0.4116950093476029 0.4971669207202543

0.4792394489389634 0.5731464289673366 0.5301581608459679
0.4475315935554994 0.4896354181054527 0.5617286186300031
0.3424743008888028 0.7089287762771136 0.3831064257115815
0.3755863357601767 0.7601253924420333 0.5451172067089262
0.4327859702799562 0.4689109905818601 0.4907290046904564
0.4648151149276774 0.5516497413150312 0.4597710057512412
0.2601367704798135 0.4590612771797872 0.6604121740287897
0.5695454020620021 0.5342009925764565 0.5203068254048004
0.5372799162380424 0.4514369111503172 0.5528998049380796
0.5199985275720527 0.4314111351171175 0.4822992342389122
0.5520538929949167 0.5133467098563768 0.4499383114409297
0.7342319669918302 0.5380351863770846 0.3431303403971631
0.7228053268759840 0.6000063319313864 0.5530023422032897
0.7757219587143902 0.5891572363207082 0.5030749952768802
0.5733439909029576 0.2866247931904402 0.4187400598684149
0.6241132969487517 0.2478722638943811 0.4554475422309368
0.6592850127751715 0.2889502034254951 0.6199998126849755
0.6233494238960813 0.3444575881641044 0.6523004688624264
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0.6249197627174679 0.5416835234935642 0.4641003021282883
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0.6557658361548838 0.5587161525035810 0.4947576066589928
0.5667597056365740 0.3520734436833348 0.4903068335047571

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0.6807075453768237	0.5439569467132119	0.4042275421962657
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0.6084379357490500	0.3315976739833568	0.5729495785205050
0.6923129091241991	0.5361368107115939	0.3595029384782528
0.7122291704289632	0.5618240068007406	0.4351588520194319
0.7315999480168107	0.5855411403425359	0.5113697636023899
0.5961210829948732	0.2831092739304057	0.4574046926062654
0.6120494666780002	0.3015115732189499	0.5361068592990071
0.6294627506115363	0.3221256410021312	0.6137690515876564
0.4880210037586682	0.5799672664934556	0.5914171872126185
0.3852090341248139	0.4818940158772472	0.6124828498090422
0.3581371089339545	0.4431615961171207	0.4784115617372344
0.4193585732692700	0.6028345955838922	0.4174085352516417
0.4478741424886223	0.6463278393667058	0.5502642872834768
0.2555686527240525	0.4237893338079528	0.5799648595020981
0.3757653665434872	0.7348798024478966	0.4607449038986922
0.6119344283995967	0.5184896302166747	0.3980803389804310
0.6453021840160258	0.5616844320996542	0.5294443703679782
0.5520631220352960	0.3626689194687269	0.4587788410337883
0.5810903808105981	0.3967902371240785	0.5937477836663787
0.7434913241261335	0.5758541396288509	0.4226497496606690
0.6252542400483304	0.2679890991533495	0.5417425286075443
0.3307871642443426	0.7201283565165814	0.4113502370811761
0.2182794437116147	0.4292670696799525	0.5229992184635326
0.4052570205984594	0.6328649522541088	0.3600717858822632
0.3156840804233118	0.4024115925554407	0.4483072920712285
0.5491488615852694	0.3079371960527016	0.4230701717928789
0.7549273534128332	0.5360848557944249	0.3681618196269271
0.6465747433305191	0.2514325267104424	0.4787388853531656
0.5977752186085755	0.3643186125892225	0.6490379367765289
0.6702689414509608	0.2796222581594099	0.5908030857935105
0.7827057858584109	0.5702404395007525	0.4775056820875563
0.6906077581959977	0.6027564505443560	0.5567458342285936
0.3603567852781861	0.4691328041333450	0.6722106750433249
0.2407775990439705	0.4606175600239147	0.6342867223527103
0.3534245395506319	0.7546518906954758	0.5218976333100205
0.4526047697347345	0.7057160943221263	0.5818531025495567
0.6333087147839813	0.5304719605715441	0.3374881962187667

Au*-Cu

1.0000000000000000

30.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 30.0000000000000000 0.0000000000000000

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Au Cu O C Li H
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Direct

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0.2798449201113011	0.4007991526501111	0.4417049848697241
0.3814265594019332	0.6475400570158346	0.3518995805718017
0.4217185085434351	0.7282106229444389	0.5796735269090521
0.2216469067703714	0.4076607788658962	0.4860526530529490
0.4744128251044511	0.5780591340708496	0.5354571168189266
0.4374857308908577	0.4669512882522137	0.5732682398426573
0.3430717115736344	0.7051018257365080	0.3766720547235654
0.3733566039093802	0.7640166766625608	0.5377485288925780
0.4308663995341334	0.4761480597221419	0.4977808449119578
0.4691603526327953	0.5540460294025343	0.4637757392003744
0.2457735674952845	0.4532334656445614	0.6519872643301087
0.5796049929326450	0.5512239371747870	0.5165057174856121
0.5639829680146632	0.4581291162402381	0.5493508479444388
0.5186781573955742	0.4371647618793139	0.4924144841147310
0.5566201813011454	0.5149534820831577	0.4543090373750273
0.7343535628186176	0.5338006467381510	0.3312342098096408
0.7335816719799420	0.6016715603077217	0.5393110164822024
0.7848503138676988	0.5883853870180039	0.4884325246744922
0.5681947276684430	0.2894593710565981	0.4153017413743339
0.6181833601368958	0.2481073971833549	0.4500143575739644
0.6569199535791067	0.2818588862780727	0.6159349346574245
0.6252522695640748	0.3398060115541802	0.6481580394458919
0.6627424439121369	0.5233020734878461	0.3183478025524237
0.5716309463185013	0.5408542902681930	0.6257079269335150
0.5288955822591834	0.5371742811246324	0.6404793603201603
0.2888262273772194	0.4570108067101215	0.6395401595831558
0.2661668467874277	0.4133401590191193	0.4825715186179678
0.3729638201511778	0.6733322037225852	0.3875660152994558
0.4004956878294407	0.7283488278035830	0.5403606168944134
0.4623598112450606	0.5821831911231210	0.4958719146800850
0.4160223936548467	0.4674401405542071	0.5361040797872334
0.3500618752679095	0.4611158250965650	0.5854985532166428
0.3397098620074547	0.4409692835757709	0.5079528886045402
0.4178816573854207	0.6292330903934353	0.4406564975212511
0.4303743537365221	0.6562603948058299	0.5156020113537614
0.2771223478188005	0.4343579977042575	0.5609838977730519
0.3869862369479930	0.7016799518505810	0.4633968135159694
0.3047969788474083	0.4511062230498167	0.5956837957625516
0.2940457518760885	0.4296082800346945	0.5167727868018602
0.3923470185635142	0.6681376446074921	0.4301801874177817

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0.5676475691681032 0.3836067820355348 0.5247846627676505
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0.7409617250136917 0.5861332154143838 0.4979926357210245
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0.3536033495147459 0.4397749236466230 0.4742969580986933
0.4221094337818616 0.6018458186009890 0.4170013836549613
0.4442714579203006 0.6483865562490151 0.5483780085517881
0.2445526402301960 0.4202143381546498 0.5693258227045156
0.3729249418842556 0.7340285812317822 0.4540404991502587
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0.6540970885821865 0.5682895846454901 0.5191882412627409
0.5515464226458346 0.3665946289562552 0.4576922179933718
0.5903722146195294 0.3968372299097102 0.5904636456827270
0.7489834651476022 0.5717391210976317 0.4089565860439990
0.6212445250436280 0.2652936211222826 0.5358735327762194
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0.2271672116868537 0.4542995763773644 0.6253649522852341
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0.6330972321218257 0.5284312404520889 0.3308129864197155

Cu*-Pt

1.0000000000000000
30.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000

Pt Cu O C Li H
1 1 26 36 1 28

Direct

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0.3814265594019332 0.6475400570158346 0.3518995805718017
0.4217185085434351 0.7282106229444389 0.5796735269090521
0.2216469067703714 0.4076607788658962 0.4860526530529490
0.4744128251044511 0.5780591340708496 0.5354571168189266
0.4374857308908577 0.4669512882522137 0.5732682398426573
0.3430717115736344 0.7051018257365080 0.3766720547235654
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0.6207198129651442 0.2682542785571216 0.5346028030997272
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Pt*-Mo DMSC

1.0000000000000000

30.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000

Pt Mo O C Li H
1 1 26 36 1 28

Direct

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Re*-Mo

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0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000

Re Mo O C Li H

1 1 26 36 1 28

Direct

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0.2234531232719727 0.4095347336722662 0.4931886577374402
0.4757637378014316 0.5735060352931353 0.5269224811144415
0.4427941949056222 0.4882098339159634 0.5583126434823055
0.3404718021582681 0.7097147129438004 0.3792246442447756
0.3746399049086732 0.7600448461951896 0.5414469293725038
0.4307019614710215 0.4679268467624823 0.4870324339761644
0.4637114960994416 0.5513426829432770 0.4561914496531134
0.2573191903665688 0.4575735754584561 0.6564807432074347
0.5701389471798980 0.5358509370104987 0.5182034505000114
0.5344576810374216 0.4485194106222671 0.5510042787796551
0.5201483033704025 0.4304588537329693 0.4795357634920950
0.5529345435901469 0.5140149298472011 0.4487720420358588
0.7333987433364222 0.5364933849272997 0.3390900515601593
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0.7783365759284960 0.5878150544652311 0.4980905428678500
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0.6590887179560199 0.2869169155484728 0.6161649904819829
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0.4029449689414645	0.6337485339825611	0.3546145937347622
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0.6699313107353410	0.2779350766393001	0.5868115562698140
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0.6939868242828801	0.6063401606415638	0.5507797722433819
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Ru*-Pd

1.0000000000000000

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0.0000000000000000 30.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

Pd Ru O C H

1 1 24 36 28

Direct

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Ru*-Pt

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Pd Ru O C H
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Nb*-Mo

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Mo*-Pt DMSC

1.0000000000000000

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0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000

Pt Mo O C Li H
1 1 26 36 1 28

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Fe*-Cu

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Cu Fe O C Li H
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Direct

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Ti*-Fe

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Direct

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Rh*-Re

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Re Rh O C Li H

1 1 26 36 1 28

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Ta*-Ta

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2 26 36 1 28

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Re*-Rh

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Re Rh O C Li H

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References:

- (1) G. Kresse, J. Hafner, *Phys. Rev. B: Condens. Matter Mater. Phys.* 1994, **49**, 14251.
- (2) G. Kresse, D. Joubert, *Phys. Rev. B* 1999, **59**, 1758.
- (3) J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* 1996, **77**, 3865.
- (4) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104.
- (5) G. Henkelman, A. Arnaldsson, H. Jónsson, *Comput. Mater. Sci.* 2006, **36**, 354–360.